



SCIENTIFIC PROGRAM

September 7, Thursday

18⁰⁰-20⁰⁰ Arrival and Registration in New Peterhof Hotel, St.Petersburg, Russia
Welcome Party

September 8, Friday (Hotel "New Peterhof", St.Petersburg)

09⁰⁰-09³⁰ Registration in Hotel "New Peterhof" (cont.)

09³⁰-10⁰⁰ **Opening ceremony. Welcoming by the Andrey L. Konevega** Petersburg Nuclear Physics Institute (PNPI) of the National Research Center "Kurchatov Institute" (NRC "Kurchatov Institute")

(Session I. Co-Chairs Kh. Kholmurodov & A. Shvetsov)

10⁰⁰-11⁰⁰ **Yuko Okamoto** (Nagoya University, Japan)

"Generalized-ensemble algorithms for materials and biomolecular simulations"

11⁰⁰-11³⁰ **Gennady Makarov** (South Ural State University, Chelyabinsk, Russia).

"Investigation of nascent peptide exit tunnel by means of molecular dynamics simulations"

11³⁰-12⁰⁰ **Coffee Break**

(Session II. Co-Chairs Y. Okamoto & M. Kiselev)

12⁰⁰-12³⁰ **Tomobe Katsufumi** (Keio University, Japan)

"Molecular dynamics simulation of Rhodopsin and Opsin: Water transport through internal water pathways"

12³⁰-13⁰⁰ **Andrey S. Kuznetsov** (National Research University Higher School of Economics, Myasnitskaya ul.20, 101000 Moscow, Russia)

"Structure and Function of Human Neuraminidase-1 Revisited: a Molecular Modeling Study"

13⁰⁰-14⁰⁰ **Lunch**

(Session III. Co-Chairs A. Kuznetsov & T. Katsufumi)

14⁰⁰-15⁰⁰ **Robert J. Woods** (Complex Carbohydrate Research Center, University of Georgia, Athens, USA)

"How Proteins Recognize Flexible Carbohydrates: The Roles of Affinity, Avidity, and Entropy"

15⁰⁰-15³⁰ **Anton O. Chugunov** (National Research University Higher School of Economics, Myasnitskaya ul.20, 101000 Moscow, Russia)

"Temperature-sensing receptor TRPV1: mechanism of gating as revealed by computation"

15³⁰-16⁰⁰ **Alexei Shvetsov** (PNPI, NRC "Kurchatov Institute", St.Petersburg, Russian Federation).

"New computational method to get D2O/H2O contrast from all-atom molecular dynamics trajectories for large biomacromolecular complexes"

16⁰⁰-16³⁰ **Coffee Break**

(Session IV. Co-Chairs R. Woods & R. Efremov)

16³⁰-17³⁰ **Dmitry Lebedev** (PNPI, NRC "Kurchatov Institute", St.Petersburg, Russian Federation).

"Prospects for the Life Science Research at the Russian Science Mega-Project Neutron Source Reactor PIK"

17³⁰-18⁰⁰ **Norbert Kucerka** (Frank Laboratory of Neutron Physics, JINR, Dubna, Russian Federation).

"Peculiar properties of lipid membranes by neutron diffraction"

18⁰⁰-18³⁰ **Georgy Rychkov** (PNPI, NRC "Kurchatov Institute", St.Petersburg, Russian Federation).

"Partially assembled nucleosome structures: full-atom molecular models and experimental data interpretation"

18³⁰-19⁰⁰ **Kholmirzo Kholmurodov** (Frank Laboratory of Neutron Physics, JINR, Dubna, Russian Federation).

"Computer molecular dynamics of nanoscale phenomena: exploring new drugs and materials"

Closing of the 1st conference day



September 9, Saturday (Hotel "New Peterhof", St.Petersburg)

(Session V. Co-Chairs J. Golebiowski, Pr. & Kh. Kholmurodov)

09⁰⁰-10⁰⁰ **Roman Efremov** (National Research University Higher School of Economics, Myasnitskaya ul.20, 101000 Moscow, Russia).

"Principles of molecular recognition in cell membranes: a computational view"

10⁰⁰-10³⁰ **Mikhail Kiselev** (Frank Laboratory of Neutron Physics, JINR, Dubna, Russian Federation).

"SANS study of unilamellar DMPC vesicles: Fluctuation model of a lipid bilayer"

10³⁰-11⁰⁰ **Coffee Break**

(Session VI. Co-Chairs A. Chugunov & N. Kucerka)

11⁰⁰-12⁰⁰ **Jérôme Golebiowski, Pr.** (University Nice Sophia Antipolis, Nice, France).

"Smelling in silico"

12⁰⁰-12³⁰ **Michael Petukhov** (PNPI, NRC "Kurchatov Institute", St.Petersburg, Russian Federation).

"Design of stable α -helical peptides for biotechnology and medicine"

12³⁰-12⁵⁰ **Eric Dushanov** (Laboratory of Radiation Biology, JINR, Dubna, Russian Federation).

"Cation-containing lipid membranes – experiment and md simulations"

12⁵⁰-13⁰⁰ **Khaiyom Rahmonov** (Academy of Science, Dushanbe, Republic of Tajikistan).

"Molecular Dynamics Simulations and In Situ Small Angle Neutron Scattering on Electrolyte Density Distribution of Lithium–Air Battery"

13⁰⁰-14⁰⁰ **Lunch**

(Session VII. Co-Chairs A. Konevega & Kh. Kholmurodov)

14⁰⁰-15⁰⁰ **Tomoyuki Yamamoto** (Waseda University, Japan).

"XANES analysis for functional materials"

15⁰⁰-15³⁰ **Mekhrdod Subhoni** (Physical Technical institute named after S. Umarov of Academy of Sciences of the Republic of Tajikistan).

"Experimental and DFT studies of the Mn-doped CaTiO₃, CaZrO₃, CaHfO₃ and CaSnO₃"

15³⁰-16⁰⁰ **Andrey Gurtovenko** (Institute of Macromolecular Compounds, Russian Academy of Sciences, St.Petersburg, Russia).

"Computer modeling of DNA delivery vectors"

16⁰⁰-16³⁰ **Vladimir Fedorov** (Biological Faculty, Moscow State University)

"Electron-transfer protein-protein complex formation in higher plants and cyanobacteria"

16³⁰-17⁰⁰ **Vladimir Egorov** (PNPI, NRC "Kurchatov Institute", St.Petersburg, Russian Federation)

"Molecular dynamics modeling of triazavirine anti-amyloidogenic action mechanism"

17⁰⁰-17³⁰ **Round table with Coffee Break. Symposium Closing.**

18⁰⁰-22³⁰ **Social program** (excursion to be conducted in English with start and finish at the hotel New Peterhof)

September 10, Sunday (Hotel "New Peterhof", St.Petersburg)

Departure of the MSSMBS'17' delegates